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Conspicuous current dependence of the emission energy from $In_xGa_{1-x}N$/GaN quantum well diodes

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ABSTRACT

The emission spectrum of the conventional InGaN/GaN quantum well (QW) diode changes remarkably with the operating current. The degree of change depends on the constituent parameters of the QW. A detailed investigation has been carried out through the self-consistent solutions of the Schrödinger and Poisson equations to elucidate the change of the emission energy and the transition probability with the operating current and to explore how the changes depend on the well width of the QW and the In mole fraction. It is found that choosing suitable values of the mentioned parameters, the emission energy may be kept almost constant with current, or it may be tuned over a wide range through current. The two possibilities have immense importance for optoelectronic device applications.

1. Introduction

InGaN based quantum wells (QWs) are highly promising material systems for light emitting diodes (LEDs) and laser diodes (LDs) in visible and ultraviolet range. In spite of high defect and dislocation density in the InGaN epilayers significantly large intensity emission is obtained from InGaN based QW light emitting devices [1,2]. One of the major challenges faced by the conventional (*c*-plain) InGaN QW lighting devices is a strong blue shift in the emission wavelength with increase in the operating current [3–5]. The phenomenon is attributed to the presence of a huge internal electrostatic field, produced by the large piezoelectric and spontaneous polarization [4,6], though detailed quantitative discussions seem still inadequate.

Group III-nitrides, having wurtzite structure, possess large piezoelectric coefficients and spontaneous polarization [6]. The lattice mismatch between GaN and InN gives rise to a large amount of misfit strain in the InGaN QW layer depending on the In mole fraction. The strain, in turn, leads to large piezoelectric polarization in the QW. The abrupt changes of the piezoelectric and spontaneous polarization at the hetero-interfaces produce a huge polarization field.

The influence of the polarization field on the transition energy of the QW structures can be controlled effectively by the fundamental parameters of the structures, like width of the QW, In composition and the doping density in the barrier [6,7]. We have reported the effect of doping concentration on the emission energy of InGan/GaN QW diodes in detail [8].

Although the shift of the emission peak with current in InGaN QW based LEDs and LDs below the threshold current, has been reported in several literature, detailed study of its dependence on the different fundamental parameters of the structures seems required.

In this paper we explore in detail how the shift of the emission peak with the operating current in InGaN/GaN QW diodes depends on the fundamental parameters, the width of the QW and the In mole fraction. The field distribution and the energy band profile for each case have been studied alongside. With increase in the width of the QW, the emission peak energy decreases widely but its change with the operating current enhances drastically. In each case the change in the emission energy is much more for higher In content. The transition probability i.e. the square of the overlap of electron and hole wave functions has been computed in each case to determine the radiative recombination rate. The effect of the doping concentration, published previously, on the emission energy is also briefly discussed for comprehensive understanding [8].

These investigations reveal the basic features of InGaN/GaN QW lighting devices for more stable emission and will be useful in designing such devices with better accuracy. The development of modern white LEDs and multicolour LEDs, having multiple QWs with different emission wave lengths, can also be benefited from these studies. Moreover, these studies will be helpful to illuminate a very important feature, the current tunability of the emission energy in such diodes choosing appropriate parameters [9].

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2. Theoretical details

The model structure used for calculations is a GaN pn junction diode which consists of an $In_xGa_{1-x}N$ single QW at the junction. At room temperature the band gap of $In_xGa_{1-x}N$ is calculated using the interpolation method [10] considering the band gap of GaN and InN 3.43 [11] and 0.7 eV [12] respectively and the bowing parameter 1.4 eV [10]. In our calculations the ratio of conduction band and valance band offset is consider to be 68:32 [13]. Other material parameters, used in the calculations, are taken from [10]. The spontaneous polarization in GaN and $In_xGa_{1-x}N$, and the piezoelectric polarization in the strained $In_xGa_{1-x}N$ layer is calculated using the expressions, developed by Fiorentini et al. [14].

The electron and hole distribution in the structure are computed by solving the Schrödinger and Poisson equations self-consistently using the finite difference method with non-uniform mesh. The details of the calculations have been discussed elaborately in our published article [8].

The overlap of electron and hole wave functions is derived from the definition [15]

$$M_{eh} = \int_{-\infty}^{+\infty} \psi_e \psi_h \, dz \tag{1}$$

and the transition probability is given by M_{eh}^2.

The current density through the diode is determined from the relation [16,17]

$$J = qd(U_{SHR} + U_{b-b} + U_A), \tag{2}$$

where U_{SHR} is the Shockley–Hall–Read (SHR) recombination rate, $U_{b\text{-}b}$ is the band to band or radiative recombination rate, U_A is the Auger recombination rate, d is the width of the QW and q is the electronic charge. For high level injection the recombination rates can be approximated as [16]

$$U_A = \frac{1}{2} C_a n_w p_w (n_w + p_w), \tag{3}$$

$$U_{b-b} = R_{sp} n_w p_w \tag{4}$$

and

$$U_{SHR} = A_{nr} n_w, \tag{5}$$

where C_a is the Auger recombination coefficient, R_{sp} is the radiative recombination coefficient, A_{nr} is the SHR coefficient, n_w is the electron concentration and p_w is the hole concentration in the QW. C_a and A_{nr} are considered to be $1.5 \times 10^{-30}\ cm^6\ s^{-1}$ and $10^7\ s^{-1}$ respectively [17,18]. R_{sp} is proportional to the square of the transition matrix element which in turn, is proportional to M_{eh} [19,20]. In presence of the large polarization field in the QW, M_{eh} is significantly affected by the operating current and the fundamental parameters of the structure. So instead of taking any constant value of R_{sp}, it is expressed as

$$R_{sp} = M_{eh}^2 K, \tag{6}$$

and K is determined by comparing Eq. (6) with the reported value [17,18] of R_{sp} for a particular structure.

3. Results and discussion

The variation of the lowest interband transition energy with the current density for different widths of the QW at two widely different In compositions, is shown in Fig. 1. The n-type and p-type doping concentrations in the GaN barriers are kept at $5 \times 10^{18}\ cm^{-3}$. The variation of the transition probability in each case is given along side. As depicted in the figure, the transition energy increases gradually with the operating current and the rate of increment is higher for wider QWs and higher In mole fractions. For 2 nm QWs the

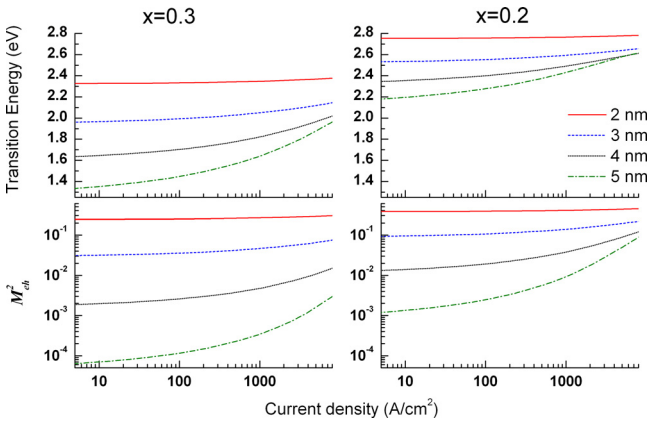

Fig. 1. Transition energy and transition probability as a function of current density for different well widths at two different In compositions.

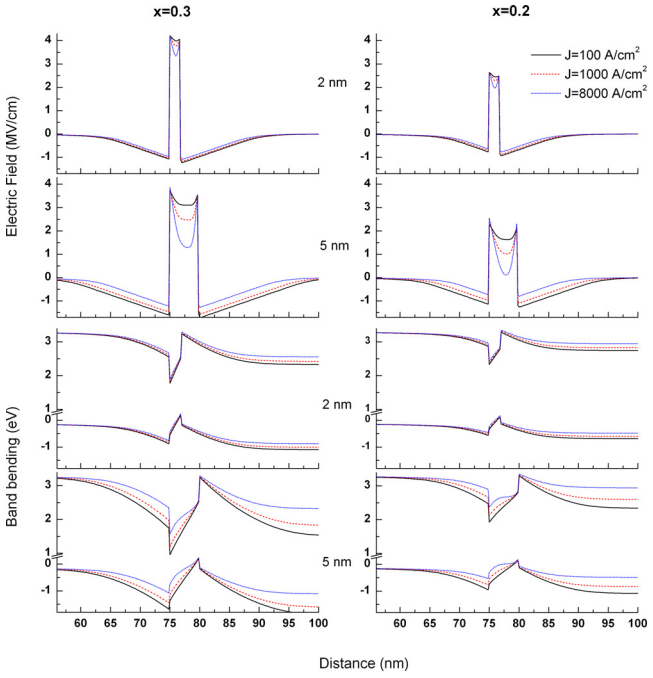

Fig. 2. Electric field distribution and band profile in and around the QW for different current densities at two widely different well widths and different In mole fractions.

increase in the transition energy is not monotonic when the forward current is very low, though the change in the overall transition energy is very small. It is seen that there is a large red shift of the transition energy as the well width increases and this red shift is much more for higher In content.

It is observed that as the well becomes wider the transition probability decreases drastically but its change with operating current increases. For higher In mole fractions the transition probability reduces further and its changes with the current density and with the width of the well become much more.

To explain these observations the electric field distribution and the band profile of the structure have been computed for different current densities and two different well widths with different In compositions are shown in Fig. 2. The electric field has three components which arise from three different mechanisms. These are the pn junction field (F_{pn}), the field due to excess carriers (F_{ex}) and the polarization field (F_p). We have discussed in Ref. [8] how these field components arise, interact and are influenced by the operating current. The components are shown schematically in Fig. 3. F_{pn} and